

ORGANOMETALLICS

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Table 3. Bond lengths [Å] and angles [°] for 96259.

Fe(1)-N(1)	1.951(6)	Fe(1)-P(2)	2.330(2)
Fe(1)-P(1)	2.350(2)	Fe(1)-Br(1)	2.4201(13)
Fe(1)-Br(2)	2.4263(12)	P(1)-C(13)	1.807(8)
P(1)-C(7)	1.831(8)	P(1)-C(1)	1.844(7)
C(1)-C(6)	1.375(11)	C(1)-C(2)	1.392(11)
C(2)-C(3)	1.400(12)	C(3)-C(4)	1.410(13)
C(4)-C(5)	1.360(13)	C(5)-C(6)	1.382(12)
C(7)-C(12)	1.379(11)	C(7)-C(8)	1.396(11)
C(8)-C(9)	1.411(12)	C(9)-C(10)	1.364(14)
C(10)-C(11)	1.371(14)	C(11)-C(12)	1.418(12)
C(13)-Si(1)	1.903(8)	Si(1)-N(1)	1.735(6)
Si(1)-C(14)	1.885(8)	Si(1)-C(15)	1.893(9)
N(1)-Si(2)	1.743(6)	Si(2)-C(17)	1.863(8)
Si(2)-C(16)	1.890(8)	Si(2)-C(18)	1.916(8)
C(18)-P(2)	1.809(7)	P(2)-C(19)	1.806(7)
P(2)-C(25)	1.837(7)	C(19)-C(20)	1.405(10)
C(19)-C(24)	1.412(10)	C(20)-C(21)	1.380(11)
C(21)-C(22)	1.361(12)	C(22)-C(23)	1.393(12)
C(23)-C(24)	1.390(11)	C(25)-C(26)	1.397(10)
C(25)-C(30)	1.409(10)	C(26)-C(27)	1.378(10)
C(27)-C(28)	1.377(12)	C(28)-C(29)	1.406(12)
C(29)-C(30)	1.362(11)	C(31)-C(36)	1.39(2)
C(31)-C(32)	1.42(2)	C(32)-C(33)	1.40(2)
C(33)-C(34)	1.38(2)	C(34)-C(35)	1.40(2)
C(35)-C(36)	1.40(2)		
N(1)-Fe(1)-P(2)	86.9(2)	N(1)-Fe(1)-P(1)	87.3(2)
P(2)-Fe(1)-P(1)	173.35(8)	N(1)-Fe(1)-Br(1)	122.8(2)
P(2)-Fe(1)-Br(1)	91.66(6)	P(1)-Fe(1)-Br(1)	88.88(6)
N(1)-Fe(1)-Br(2)	121.0(2)	P(2)-Fe(1)-Br(2)	88.12(6)
P(1)-Fe(1)-Br(2)	97.60(6)	Br(1)-Fe(1)-Br(2)	116.10(5)
C(13)-P(1)-C(7)	109.9(4)	C(13)-P(1)-C(1)	106.4(4)
C(7)-P(1)-C(1)	101.3(3)	C(13)-P(1)-Fe(1)	99.4(3)
C(7)-P(1)-Fe(1)	118.5(3)	C(1)-P(1)-Fe(1)	120.7(2)
C(6)-C(1)-C(2)	118.9(7)	C(6)-C(1)-P(1)	119.3(6)
C(2)-C(1)-P(1)	121.7(6)	C(1)-C(2)-C(3)	120.3(8)
C(2)-C(3)-C(4)	119.3(9)	C(5)-C(4)-C(3)	119.3(8)
C(4)-C(5)-C(6)	121.0(9)	C(1)-C(6)-C(5)	121.1(8)
C(12)-C(7)-C(8)	120.8(8)	C(12)-C(7)-P(1)	120.8(6)
C(8)-C(7)-P(1)	118.4(6)	C(7)-C(8)-C(9)	118.3(8)
C(10)-C(9)-C(8)	121.0(9)	C(9)-C(10)-C(11)	120.7(9)
C(10)-C(11)-C(12)	119.8(9)	C(7)-C(12)-C(11)	119.4(9)
P(1)-C(13)-Si(1)	107.5(4)	N(1)-Si(1)-C(14)	113.2(3)
N(1)-Si(1)-C(15)	111.5(4)	C(14)-Si(1)-C(15)	109.9(4)
N(1)-Si(1)-C(13)	105.3(3)	C(14)-Si(1)-C(13)	107.8(4)
C(15)-Si(1)-C(13)	109.0(4)	Si(1)-N(1)-Si(2)	125.5(3)
Si(1)-N(1)-Fe(1)	118.2(3)	Si(2)-N(1)-Fe(1)	116.1(3)
N(1)-Si(2)-C(17)	113.1(4)	N(1)-Si(2)-C(16)	113.2(3)
C(17)-Si(2)-C(16)	107.9(4)	N(1)-Si(2)-C(18)	105.6(3)
C(17)-Si(2)-C(18)	107.4(4)	C(16)-Si(2)-C(18)	109.5(4)
P(2)-C(18)-Si(2)	108.3(4)	C(19)-P(2)-C(18)	109.1(3)
C(19)-P(2)-C(25)	103.4(3)	C(18)-P(2)-C(25)	107.7(3)
C(19)-P(2)-Fe(1)	119.6(2)	C(18)-P(2)-Fe(1)	103.0(2)
C(25)-P(2)-Fe(1)	113.6(2)	C(20)-C(19)-C(24)	118.1(7)
C(20)-C(19)-P(2)	122.2(6)	C(24)-C(19)-P(2)	119.6(6)
C(21)-C(20)-C(19)	119.7(8)	C(22)-C(21)-C(20)	121.6(8)
C(21)-C(22)-C(23)	120.6(8)	C(24)-C(23)-C(22)	118.8(8)
C(23)-C(24)-C(19)	121.0(8)	C(26)-C(25)-C(30)	118.2(7)
C(26)-C(25)-P(2)	119.5(6)	C(30)-C(25)-P(2)	122.2(6)

C(27)-C(26)-C(25)	120.9(8)	C(28)-C(27)-C(26)	120.6(8)
C(27)-C(28)-C(29)	118.9(8)	C(30)-C(29)-C(28)	120.9(8)
C(29)-C(30)-C(25)	120.4(8)	C(36)-C(31)-C(32)	117.0(12)
C(33)-C(32)-C(31)	120.4(13)	C(34)-C(33)-C(32)	121.8(13)
C(33)-C(34)-C(35)	118.6(12)	C(34)-C(35)-C(36)	120.5(14)
C(31)-C(36)-C(35)	121.8(13)		

Symmetry transformations used to generate equivalent atoms:

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Table 4. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for 96259. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [(h a)^2 U_{11} + \dots + 2 h k a b U_{12}]$

	U11	U22	U33	U23	U13	U12
Fe(1)	23(1)	23(1)	9(1)	9(1)	-1(1)	6(1)
Br(1)	51(1)	39(1)	18(1)	6(1)	-3(1)	-2(1)
Br(2)	32(1)	45(1)	40(1)	18(1)	-3(1)	9(1)
P(1)	28(1)	26(1)	10(1)	11(1)	0(1)	6(1)
C(1)	28(4)	20(4)	21(4)	8(3)	-1(3)	2(3)
C(2)	56(6)	28(5)	35(5)	11(4)	-10(4)	6(4)
C(3)	57(6)	36(6)	55(7)	9(5)	-16(5)	-1(5)
C(4)	43(5)	24(5)	43(6)	-8(4)	16(4)	-8(4)
C(5)	93(8)	37(6)	25(5)	19(4)	3(5)	-8(5)
C(6)	62(6)	40(5)	26(5)	20(4)	-4(4)	-4(5)
C(7)	41(5)	28(4)	12(4)	9(3)	6(3)	8(4)
C(8)	52(5)	30(5)	24(5)	13(4)	7(4)	15(4)
C(9)	65(7)	43(6)	47(7)	17(5)	35(5)	26(5)
C(10)	101(9)	39(6)	22(5)	2(4)	24(6)	15(6)
C(11)	91(8)	60(7)	16(5)	9(5)	6(5)	23(6)
C(12)	51(5)	46(5)	17(5)	9(4)	4(4)	1(4)
C(13)	36(5)	38(5)	24(5)	14(4)	-5(4)	13(4)
Si(1)	31(1)	31(1)	18(1)	12(1)	0(1)	13(1)
C(14)	32(5)	64(7)	50(6)	33(5)	3(4)	18(5)
C(15)	72(7)	46(6)	26(5)	19(4)	-2(4)	16(5)
N(1)	29(3)	22(3)	13(3)	7(3)	-2(3)	14(3)
Si(2)	39(1)	25(1)	13(1)	7(1)	0(1)	7(1)
C(16)	62(6)	41(5)	21(5)	5(4)	11(4)	26(5)
C(17)	71(7)	34(5)	31(5)	10(4)	-20(5)	-7(5)
C(18)	34(4)	29(4)	13(4)	6(3)	0(3)	8(4)
P(2)	24(1)	24(1)	9(1)	8(1)	0(1)	6(1)
C(19)	23(4)	22(4)	15(4)	17(3)	-2(3)	1(3)
C(20)	38(5)	30(4)	20(4)	11(3)	0(3)	8(3)
C(21)	41(5)	44(5)	36(5)	28(4)	0(4)	14(4)
C(22)	32(5)	28(4)	57(6)	25(4)	2(4)	9(4)
C(23)	23(4)	35(5)	46(5)	3(4)	7(4)	10(4)
C(24)	32(4)	34(4)	24(4)	6(3)	1(3)	7(3)
C(25)	33(4)	33(4)	9(4)	9(3)	0(3)	6(3)
C(26)	30(4)	35(4)	28(5)	9(4)	9(4)	9(3)
C(27)	34(4)	57(5)	8(4)	3(4)	-3(3)	14(4)
C(28)	26(4)	62(5)	15(4)	9(4)	-2(3)	-7(4)
C(29)	42(5)	38(5)	31(5)	1(4)	-7(4)	-4(4)
C(30)	31(4)	34(4)	24(4)	14(4)	4(3)	5(3)
C(31)	108(17)	66(14)	69(17)	23(10)	-65(11)	26(12)
C(32)	29(13)	101(21)	75(23)	56(13)	3(12)	27(10)
C(33)	101(13)	68(13)	29(11)	14(9)	-17(9)	53(10)
C(34)	49(9)	14(8)	73(13)	14(7)	-53(8)	-2(7)
C(35)	77(14)	110(17)	55(14)	39(11)	-8(10)	56(11)
C(36)	154(27)	61(16)	7(13)	-8(11)	-20(13)	79(14)

Table 5. Torsion angles [$^{\circ}$] for 96259.

N(1)-Fe(1)-P(1)-C(13)	42.6(3)	P(2)-Fe(1)-P(1)-C(13)	14.4(8)
Br(1)-Fe(1)-P(1)-C(13)	-80.3(3)	Br(2)-Fe(1)-P(1)-C(13)	163.5(3)
N(1)-Fe(1)-P(1)-C(7)	161.5(3)	P(2)-Fe(1)-P(1)-C(7)	133.3(7)
Br(1)-Fe(1)-P(1)-C(7)	38.6(3)	Br(2)-Fe(1)-P(1)-C(7)	-77.6(3)
N(1)-Fe(1)-P(1)-C(1)	-72.9(3)	P(2)-Fe(1)-P(1)-C(1)	-101.1(7)
Br(1)-Fe(1)-P(1)-C(1)	164.2(3)	Br(2)-Fe(1)-P(1)-C(1)	48.0(3)
C(13)-P(1)-C(1)-C(6)	55.2(8)	C(7)-P(1)-C(1)-C(6)	-59.8(7)
Fe(1)-P(1)-C(1)-C(6)	167.0(6)	C(13)-P(1)-C(1)-C(2)	-129.3(7)
C(7)-P(1)-C(1)-C(2)	115.7(7)	Fe(1)-P(1)-C(1)-C(2)	-17.5(8)
C(6)-C(1)-C(2)-C(3)	0.9(13)	P(1)-C(1)-C(2)-C(3)	-174.6(7)
C(1)-C(2)-C(3)-C(4)	2.6(14)	C(2)-C(3)-C(4)-C(5)	-4.4(14)
C(3)-C(4)-C(5)-C(6)	2.9(14)	C(2)-C(1)-C(6)-C(5)	-2.6(13)
P(1)-C(1)-C(6)-C(5)	173.0(7)	C(4)-C(5)-C(6)-C(1)	1(2)
C(13)-P(1)-C(7)-C(12)	13.4(8)	C(1)-P(1)-C(7)-C(12)	125.6(7)
Fe(1)-P(1)-C(7)-C(12)	-99.9(7)	C(13)-P(1)-C(7)-C(8)	-167.2(6)
C(1)-P(1)-C(7)-C(8)	-54.9(7)	Fe(1)-P(1)-C(7)-C(8)	79.6(6)
C(12)-C(7)-C(8)-C(9)	-0.2(12)	P(1)-C(7)-C(8)-C(9)	-179.6(6)
C(7)-C(8)-C(9)-C(10)	0.6(13)	C(8)-C(9)-C(10)-C(11)	-1(2)
C(9)-C(10)-C(11)-C(12)	1(2)	C(8)-C(7)-C(12)-C(11)	0.3(13)
P(1)-C(7)-C(12)-C(11)	179.7(7)	C(10)-C(11)-C(12)-C(7)	-0.7(14)
C(7)-P(1)-C(13)-Si(1)	-166.8(4)	C(1)-P(1)-C(13)-Si(1)	84.3(4)
Fe(1)-P(1)-C(13)-Si(1)	-41.7(4)	P(1)-C(13)-Si(1)-N(1)	22.9(5)
P(1)-C(13)-Si(1)-C(14)	144.0(4)	P(1)-C(13)-Si(1)-C(15)	-96.7(5)
C(14)-Si(1)-N(1)-Si(2)	81.1(5)	C(15)-Si(1)-N(1)-Si(2)	-43.4(6)
C(13)-Si(1)-N(1)-Si(2)	-161.5(4)	C(14)-Si(1)-N(1)-Fe(1)	-103.9(5)
C(15)-Si(1)-N(1)-Fe(1)	131.6(4)	C(13)-Si(1)-N(1)-Fe(1)	13.6(4)
P(2)-Fe(1)-N(1)-Si(1)	143.1(3)	P(1)-Fe(1)-N(1)-Si(1)	-33.8(3)
Br(1)-Fe(1)-N(1)-Si(1)	53.1(4)	Br(2)-Fe(1)-N(1)-Si(1)	-131.0(3)
P(2)-Fe(1)-N(1)-Si(2)	-41.4(3)	P(1)-Fe(1)-N(1)-Si(2)	141.7(3)
Br(1)-Fe(1)-N(1)-Si(2)	-131.4(3)	Br(2)-Fe(1)-N(1)-Si(2)	44.5(4)
Si(1)-N(1)-Si(2)-C(17)	88.0(5)	Fe(1)-N(1)-Si(2)-C(17)	-87.2(5)
Si(1)-N(1)-Si(2)-C(16)	-35.1(6)	Fe(1)-N(1)-Si(2)-C(16)	149.7(4)
Si(1)-N(1)-Si(2)-C(18)	-154.9(4)	Fe(1)-N(1)-Si(2)-C(18)	29.9(4)
N(1)-Si(2)-C(18)-P(2)	4.4(5)	C(17)-Si(2)-C(18)-P(2)	125.4(4)
C(16)-Si(2)-C(18)-P(2)	-117.8(4)	Si(2)-C(18)-P(2)-C(19)	-157.0(3)
Si(2)-C(18)-P(2)-C(25)	91.5(4)	Si(2)-C(18)-P(2)-Fe(1)	-28.9(4)
N(1)-Fe(1)-P(2)-C(19)	160.5(3)	P(1)-Fe(1)-P(2)-C(19)	-171.3(7)
Br(1)-Fe(1)-P(2)-C(19)	-76.7(3)	Br(2)-Fe(1)-P(2)-C(19)	39.4(3)
N(1)-Fe(1)-P(2)-C(18)	39.3(3)	P(1)-Fe(1)-P(2)-C(18)	67.5(8)
Br(1)-Fe(1)-P(2)-C(18)	162.1(3)	Br(2)-Fe(1)-P(2)-C(18)	-81.8(3)
N(1)-Fe(1)-P(2)-C(25)	-76.9(3)	P(1)-Fe(1)-P(2)-C(25)	-48.7(8)
Br(1)-Fe(1)-P(2)-C(25)	45.9(3)	Br(2)-Fe(1)-P(2)-C(25)	161.9(3)
C(18)-P(2)-C(19)-C(20)	-16.0(7)	C(25)-P(2)-C(19)-C(20)	98.5(6)
Fe(1)-P(2)-C(19)-C(20)	-134.1(5)	C(18)-P(2)-C(19)-C(24)	167.7(6)
C(25)-P(2)-C(19)-C(24)	-77.8(6)	Fe(1)-P(2)-C(19)-C(24)	49.7(6)
C(24)-C(19)-C(20)-C(21)	2.6(11)	P(2)-C(19)-C(20)-C(21)	-173.7(6)
C(19)-C(20)-C(21)-C(22)	0.1(12)	C(20)-C(21)-C(22)-C(23)	-1.1(12)
C(21)-C(22)-C(23)-C(24)	-0.7(12)	C(22)-C(23)-C(24)-C(19)	3.5(11)
C(20)-C(19)-C(24)-C(23)	-4.4(11)	P(2)-C(19)-C(24)-C(23)	172.0(6)
C(19)-P(2)-C(25)-C(26)	-171.3(6)	C(18)-P(2)-C(25)-C(26)	-55.9(7)
Fe(1)-P(2)-C(25)-C(26)	57.5(7)	C(19)-P(2)-C(25)-C(30)	11.6(7)
C(18)-P(2)-C(25)-C(30)	127.0(6)	Fe(1)-P(2)-C(25)-C(30)	-119.6(6)
C(30)-C(25)-C(26)-C(27)	-0.7(11)	P(2)-C(25)-C(26)-C(27)	-177.9(6)
C(25)-C(26)-C(27)-C(28)	0.7(12)	C(26)-C(27)-C(28)-C(29)	-0.6(12)
C(27)-C(28)-C(29)-C(30)	0.6(12)	C(28)-C(29)-C(30)-C(25)	-0.7(12)
C(26)-C(25)-C(30)-C(29)	0.7(11)	P(2)-C(25)-C(30)-C(29)	177.8(6)
C(36)-C(31)-C(32)-C(33)	0.0(2)	C(31)-C(32)-C(33)-C(34)	0.0(2)
C(32)-C(33)-C(34)-C(35)	0.0(2)	C(33)-C(34)-C(35)-C(36)	0.0(2)
C(32)-C(31)-C(36)-C(35)	0.0(2)	C(34)-C(35)-C(36)-C(31)	0.0(2)

Table 6. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 96259.

	x	y	z	U(eq)	SOF
H(2A)	63(9)	1391(7)	2333(6)	47	1
H(3A)	-1521(10)	-325(8)	2186(7)	60	1
H(4A)	-1562(9)	-1566(7)	3234(6)	47	1
H(5A)	134(11)	-1205(8)	4280(6)	62	1
H(6A)	1756(10)	441(7)	4384(5)	51	1
H(8A)	-300(9)	3021(7)	4228(5)	40	1
H(9A)	-977(11)	3854(8)	5545(6)	58	1
H(10A)	596(12)	4455(8)	6642(6)	64	1
H(11A)	2861(12)	4192(9)	6494(6)	65	1
H(12A)	3588(9)	3363(7)	5183(5)	45	1
H(13A)	3905(8)	1383(7)	3955(5)	37	1
H(13B)	4547(8)	2729(7)	3997(5)	37	1
H(14A)	6800(14)	2192(49)	2042(8)	68	1
H(14B)	6931(10)	1851(37)	2965(31)	68	1
H(14C)	6621(9)	3125(16)	2839(36)	68	1
H(15A)	3263(11)	-118(11)	2122(37)	69	1
H(15B)	4604(54)	-269(8)	2646(17)	69	1
H(15C)	4707(52)	-46(9)	1691(20)	69	1
H(16A)	5725(20)	2449(16)	405(31)	59	1
H(16B)	4777(18)	1527(46)	-261(8)	59	1
H(16C)	5296(35)	1143(34)	593(24)	59	1
H(17A)	1106(12)	1349(24)	700(32)	70	1
H(17B)	2079(32)	362(16)	698(32)	70	1
H(17C)	1898(39)	966(38)	-123(6)	70	1
H(18A)	3703(8)	3907(6)	104(5)	29	1
H(18B)	2111(8)	3553(6)	256(5)	29	1
H(20A)	1877(8)	5451(7)	-37(5)	34	1
H(21A)	806(8)	7039(8)	-249(6)	45	1
H(22A)	472(8)	8432(7)	843(6)	44	1
H(23A)	1167(7)	8261(7)	2215(6)	41	1
H(24A)	2145(8)	6619(7)	2464(5)	36	1
H(26A)	5828(8)	4035(7)	1539(5)	36	1
H(27A)	8068(8)	4944(8)	1707(5)	39	1
H(28A)	8560(8)	6968(8)	1831(5)	42	1
H(29A)	6758(8)	8079(8)	1753(5)	46	1
H(30A)	4527(8)	7189(7)	1586(5)	35	1
H(31A)	3931(21)	-1178(16)	4650(14)	96	0.50
H(32A)	3424(18)	177(19)	5809(14)	75	0.50
H(33A)	4942(18)	1873(14)	6242(9)	74	0.50
H(34A)	6964(15)	2286(12)	5568(10)	55	0.50
H(35A)	7481(17)	966(16)	4427(11)	89	0.50
H(36A)	5985(25)	-737(16)	3979(12)	84	0.50